Escape through an unstable limit cycle: Resonant activation

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We consider a Brownian particle acted on by a linear conservative force, a nonlinear frictional force, and multiplicative colored and additive white noises; the frictional force can be negative when the external energy supply is large enough. We numerically calculate the mean first passage time (MFPT) for the particle to escape from an unstable limit cycle and find resonant activation, i.e., the MFPT first decreases, followed by a rise after passing through a minimum with increasing noise correlation time τ for a fixed noise variance. For fixed noise strength of the multiplicative noise the MFPT increases linearly with τ. This is in sharp contrast to the case of fluctuations of nonlinear potentials, in which the MFPT first increases nonlinearly before reaching a limiting value. Our model could be useful for understanding some biological processes.

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The processes of noise-driven escape of particles over potential barriers, i.e., the well-known Kramers' problem [1], are ubiquitous in a wide variety of physical, chemical, and biological contexts [2]. Kramers considered a model Brownian particle trapped in a one-dimensional well representing the reactant state, which is separated by a barrier of finite height from a deeper well, signifying the product state. The particle was supposed to be immersed in a medium such that the medium exerts a frictional force on the particle but thermally activates it so that the particle may gain enough energy to cross the barrier. Over several decades the model and many of its variants have served as standard paradigms in various problems of physical and chemical kinetics to understand the decay rate of metastable systems in the overdamped and underdamped limits [3], the effect of anharmonicities [4], the role of the relaxing bath [5], the signature of non-Markovian effects [6], and quantum and semiclassical corrections to the classical rate and related similar aspects [7]. The vast body of literature has been the subject of several reviews [2,8]. In the majority of these studies the focus lies on the competing attractors of the dynamical system, which are separated by a separatrix containing a saddle point. However, models where the separatrix is instead an unstable limit cycle often arise in the context of chemical reactions constrained to occur far from a equilibrium [9]. The rate of escape through the unstable limit cycle in the weak noise limit has been studied [10] and noise-driven transitions in models with an unstable limit cycle can be found in Ref. [11].

Most of the works mentioned above have considered the static barrier. However, a surge of fresh interest in this topic was triggered, not long ago, by Doering and Gadoua [12] who studied how the interwell mean first passage time (MFPT) of a Brownian particle in a bistable potential depends on the correlation time τ of the barrier fluctuations. They observed that this dependence may be nonmonotonic and called it resonant activation (RA). This interesting phenomenon [12] has been further investigated [13–19]. In the present paper we examine a related issue. We show that the phenomenon of RA appears in the problem of escape through an unstable limit cycle in the presence of multiplicative colored and additive white noises. Although traditionally RA appears due to fluctuations in a nonlinear potential, the present analysis suggests that it may be observed even in the presence of a linear potential as a result of strange behavior of the limit cycle. The limit cycle is a conspicuous feature in a variety of models in biology and chemistry that deal with situations far from thermal equilibrium. On the other hand, in Refs. [17,19] it was emphasized that "far from equilibrium" is one of the necessary conditions for the RA phenomenon.

To start with, we consider a simple model defined by

$$\dot{v} = -aq + b(v^2-1)v + q\eta(t) + \zeta(t), \tag{1}$$

where q and $v \equiv \dot{q}$ represent the coordinate and the velocity of the Brownian particle, and $\eta(t)$ and $\zeta(t)$ are Gaussian colored and white noises, respectively. In general, we express the thermal fluctuation of the system as additive noise and the effect of the external environmental fluctuation on the system as multiplicative noise. Thus $\zeta(t)$ and $\eta(t)$ in Eq. (1) correspond to internal thermal noise and external noise, respectively. In a complex system multiplicative noise is very relevant and it makes the system far from equilibrium. The two noises are characterized by the relations $\langle \eta(t)\rangle=0$, $\langle \zeta(t)\rangle=0$,

$$\langle \eta(t)\eta(t')\rangle = \frac{D_0}{\tau} e^{-|t-t'|/\tau}, \tag{2}$$

$$\langle \zeta(t)\zeta(t')\rangle = 2D\delta(t-t'). \tag{3}$$

Here D_0 and τ are the strength and correlation time of the multiplicative noise; D is the strength of the additive white noise. Equation (2) shows that η in Eq. (1) is the Ornstein-

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Uhlenbeck colored noise [20]. The time evolution of η is given by

$$\dot{\eta}(t) = -\frac{\eta}{\tau} + \frac{\sqrt{D_0}}{\tau}\zeta_1, \tag{4}$$

where ζ_1 is the white Gaussian noise having variance

$$\langle \zeta_1(t)\zeta_1(t')\rangle = 2\delta(t-t'). \tag{5}$$

Some pertinent points regarding the present model may be in order. It captures essential features of barrier crossing through an unstable limit cycle in the presence of fluctuations in the activation energy. Because of the multiplicative noise term, the frequency of the linear oscillator becomes random and thereby the activation energy becomes fluctuating. The noise-driven limit cycle is a generic model for complex physical and biological processes. On the other hand, fluctuations in activation energy appear in many complex biological and physical systems. Examples include the escape of O_2 or CO ligand molecules out of a myoglobin "pocket" after photodissociation [21] and the intracellular motion of a molecular motor along a microtubule [22]; the binding of ATP and the release of ADP serve to randomly modulate the activation energy experienced by the motor protein as it travels along the biopolymer backbone. Also in other strongly coupled chemical systems [23], and even for some aspects of protein folding and relaxation in glasses, fluctuating energy barriers are likely to be of relevance [21,24]. Second, when the external energy supply is large enough, the friction (second) term in Eq. (1) becomes negative and it describes an *active* Brownian particle [25]. It stands for a simplified model of active biological motion [26]. For biological systems, an external supply of energy is crucial, e.g., to maintain metabolism and to perform movement [26]. Finally, the present model goes beyond Brownian or easy diffusive motion due to the nonlinear friction and due to being in nonequilibrium.

Without noise the model of Eq. (1) reduces to a time-reversible van der Pol oscillator. In 1996, Maier and Stein [10] calculated the white-noise-activated rate of escape through the unstable limit cycle. Now it is difficult to deal with the problem analytically because of the finite correlation of multiplicative noise and also because of the nonlinearity in velocity in Eq. (1). Therefore, we study the present problem numerically. To have the essential features of the dynamics we have solved the differential equations (1) and (4) simultaneously using Heun's method, a stochastic variant of the Euler method which reduces to the second-order Runge-Kutta method in the absence of noise [27].

Now our first task is to define the first passage time (T) for escape through an unstable limit cycle which is associated with a linear potential. To do so we plot $q(t)$ vs $v(t)$ in Fig. 1. It is apparent that if the velocity is less than -2 or greater than 2 then motion is definitely out of the attractor basin. Therefore one can define the first passage time as the time required for the particle to go from the origin of phase space (0,0) to the point where $v=2$ or $v=-2$ for the first time. Similarly one can define it in terms of the coordinate also. Since T is a statistical quantity in the presence of noise,

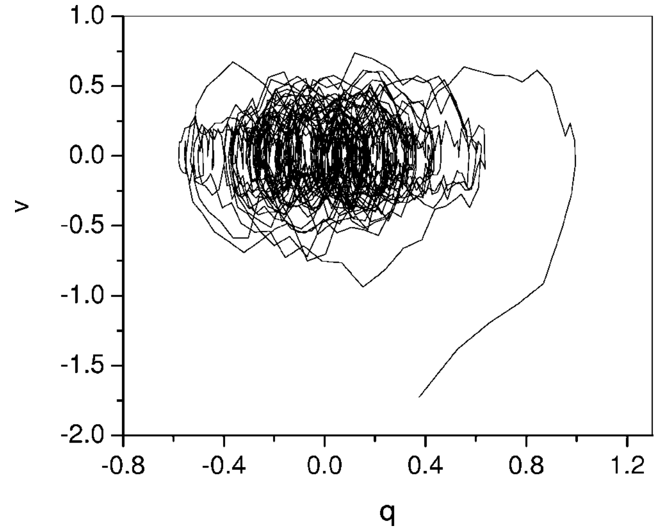

FIG. 1. Plot of the coordinate q vs the velocity v of the particle for a single realization with the parameter set $a=b=1.0$, $\tau=0.5$, $C=0.5$, and $D=0.05$ (units are arbitrary).

we calculate $\langle T\rangle$, that is, the average of T over many (say, 5000) realizations. We have calculated the MFPT for several cases. First of all, we have determined how $\langle T\rangle$ changes with increasing noise correlation time τ of multiplicative colored noise and the result is plotted in Fig. 2. To obtain data for Fig. 2, we fix the noise variance C and have

$$D_0 = C\tau. \tag{6}$$

We choose this relation with the anticipation that the nonequilibrium potential [11] in the present model might have a similar role as that of the nonlinear potential [14] in the ordinary barrier-crossing dynamics. For the nonlinear potential it was shown that RA can occur generically whenever the colored noise intensity increases sufficiently fast with in-

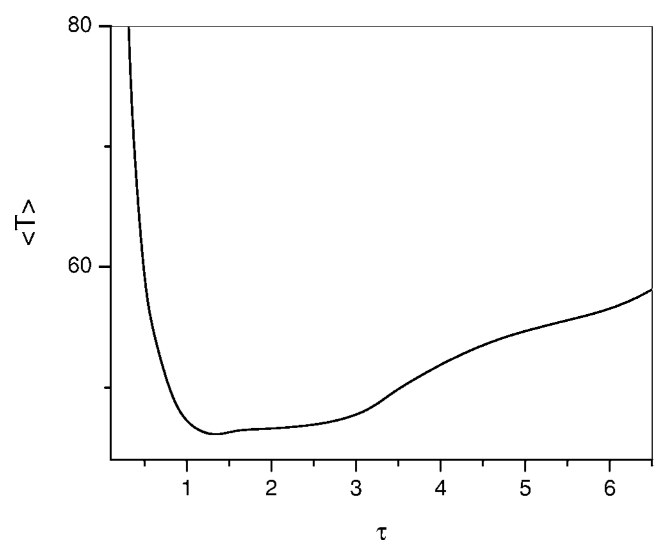

FIG. 2. Mean first passage time $\langle T\rangle$ vs the noise correlation time τ of the multiplicative colored noise with fixed noise variance for the same parameter set as in Fig. 1.

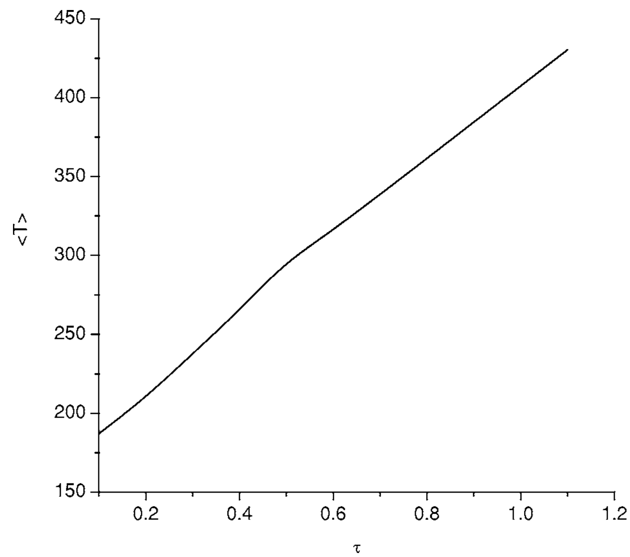

FIG. 3. Mean first passage time $\langle T\rangle$ vs the noise correlation time τ with fixed noise strength for the parameter set $a=b=1.0$, $D_0=0.1$, and $D=0.05$.

creasing τ, i.e., for a linear increase in the case when the noise variance is constant. The relation (6) has also been used in [15–18]. Figure 2 shows that the MFPT first decreases, followed by an increase after passing through a minimum. Similar results are obtained for other values of C. Thus RA is also observed for the escape of a particle through an unstable limit cycle instead of a saddle point. One important point is that we have observed RA even for a linear potential system. The feedback of energy through the nonlinear velocity-dependent term in the equation of motion plays a crucial role. It is apparent that the RA appears due to nonmonotonic behavior of the barrier height associated with the nonequilibrium potential for increase of the strength of the multiplicative noise as a linear function of the noise correlation time.

In the next step we explore how $\langle T\rangle$ changes with τ when noise strength is kept fixed. In Fig. 3, we plot $\langle T\rangle$ vs τ for a given value of D_0. The increase of $\langle T\rangle$ linearly with τ in Fig. 3 is in sharp contrast to what we observe in the calculation of the same in the case of fluctuations of nonlinear potentials. In the latter situation the MFPT first increases nonlinearly and then reaches a limiting value [17]. Thus the effect of the noise correlation time on the barrier height and the frequency factor of the rate of escape through an unstable limit cycle is different from that of escape through a saddle point.

Now we investigate the variation of $\langle T\rangle$ with strength of the multiplicative colored noise D_0. We plot the logarithm of $1/\langle T\rangle$ vs $1/D_0$ in Fig. 4 which shows that the plot is linear at small noise strength and is exponentially decaying for large values of D_0. It implies that multiplicative noise strength affects both the frequency and exponential factors of the barrier-crossing rate expression when the strength is large, and the frequency factor becomes independent of it in the weak noise limit. For additive noise our numerical experiment shows that this plot is linear (Fig. 5) for arbitrary noise strength, which is well known for the escape of a particle through a saddle point.

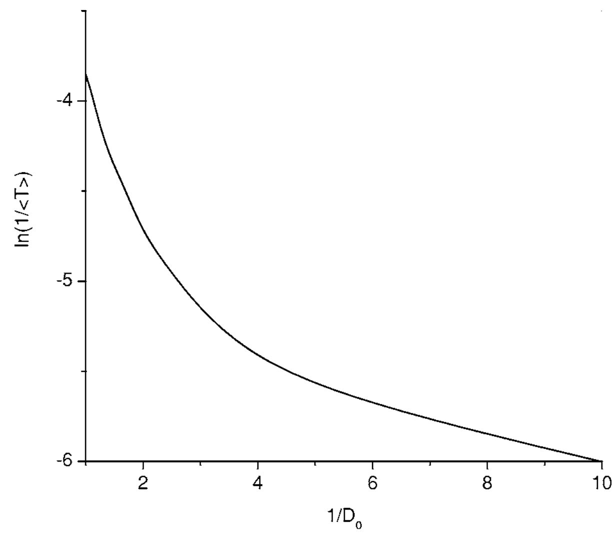

FIG. 4. $\ln(1/\langle T\rangle)$ vs $(1/D_0)$ for $a=b=\tau=1.0$ and $D=0.05$.

In summary, using a noise-driven van der Pol oscillator we have studied two aspects simultaneously: first, the escape of a Brownian particle through an unstable limit cycle in the presence of multiplicative and additive noises; second, the extraction of energy from internal thermal fluctuations as well as external fluctuations by an active Brownian particle. We have calculated here the MFPT for a Brownian particle which escapes through an unstable limit cycle from an attractor basin and found resonant activation for a given variance of the colored multiplicative noise. The essential behavior is due to the strange behavior of the limit cycle since in the present model the concerned potential is linear. From the point of view of an active Brownian particle this result implies that the energy extraction ability is first enhanced with increase of noise correlation time and then decreases after passing through a maximum for fixed variance of the multiplicative noise. We have also shown that the MFPT increases linearly with τ (thus the efficiency of the active Brownian particle decreases linearly with increasing τ) for a fixed value

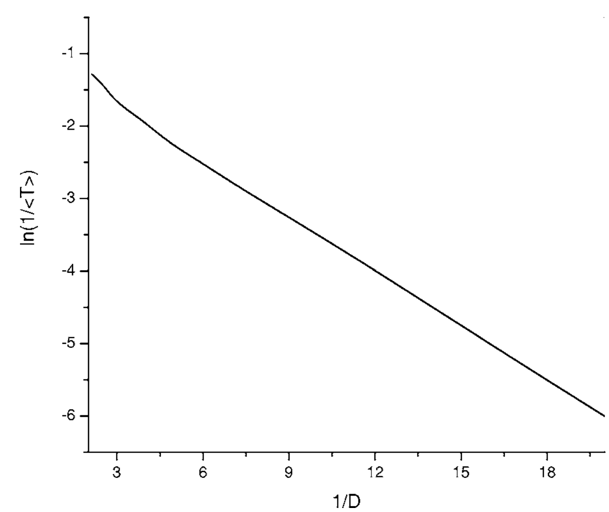

FIG. 5. $\ln(1/\langle T\rangle)$ vs $1/D$, the inverse of the strength of additive white noise for $a=b=\tau=1.0$, and $D_0=0.1$.

of the noise strength. Finally, we have shown that the strength of the multiplicative noise affects both the frequency and exponential factors at large noise strength, but the former remains unaffected as the noise strength goes to zero. Determination of the barrier-crossing rate analytically in terms of the noise correlation time and noise strength for the escape of a particle through an unstable limit cycle is an open problem for further investigation.

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